



# Getting Started with R for Mass Spectrometrists

Mass Spectrometry and Allied Topics

June 2 - 6, 2024

SHORT COURSES June 1 & 2

Anaheim

**ASMS - Short Course**



Jeff Jones, Ph. D.  
Heath Patterson, Ph. D.

#ASMS2024

# Main Topics for the Short Course

Learn ...

- basic fundamentals of the **R programming language**
- how to use to the **R Studio** integrated development environment (IDE)
- about **tidy data**, what it is, and why it's important for data analysis
- fundamentals of the **tidyverse** ecosystem of R packages and how they can be used to streamline the data analysis process
- how to make data visualizations using the **ggplot2** R package
- about some fundamental R packages for **mass spectrometry**

# The Team

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## Jeff Jones Ph.D.

Senior Scientist Proteomics, Div. Physics, Math and Astronomy, Caltech

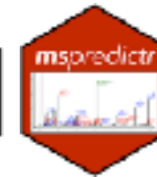
*“Started programming out of a need to analyze large data sets generated by mass spectrometry.”*

 [linkedin.com/in/jeffsocal/](https://www.linkedin.com/in/jeffsocal/)  [github.com/jeffsocal](https://github.com/jeffsocal)



[tidyproteomics jeffsocal.github.io/tidyproteomics](https://jeffsocal.github.io/tidyproteomics)

*An R package for the tidy-ing, post processing and analysis of quantitative proteomic data.*



Other  
Mass Spec.  
R Packages

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## Nathan “Heath” Patterson Ph.D.

Director of Spatial Biology Bioinformatics, Aspect Analytics, Genk, Belgium

*“Took an interest in programming when vendor solutions no longer solved the problem”*

 [linkedin.com/in/heath-patterson-a2402a100/](https://www.linkedin.com/in/heath-patterson-a2402a100/)  [github.com/nhpatterson](https://github.com/nhpatterson)

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## Ryan Benz Ph.D.

Director Data Science, Seer Inc.

*“Learning to code, even at a basic level, will open up a huge amount of new possibilities for any scientist”*

 [linkedin.com/in/ryan-benz/](https://www.linkedin.com/in/ryan-benz/)  [github.com/ZenBrayn](https://github.com/ZenBrayn)

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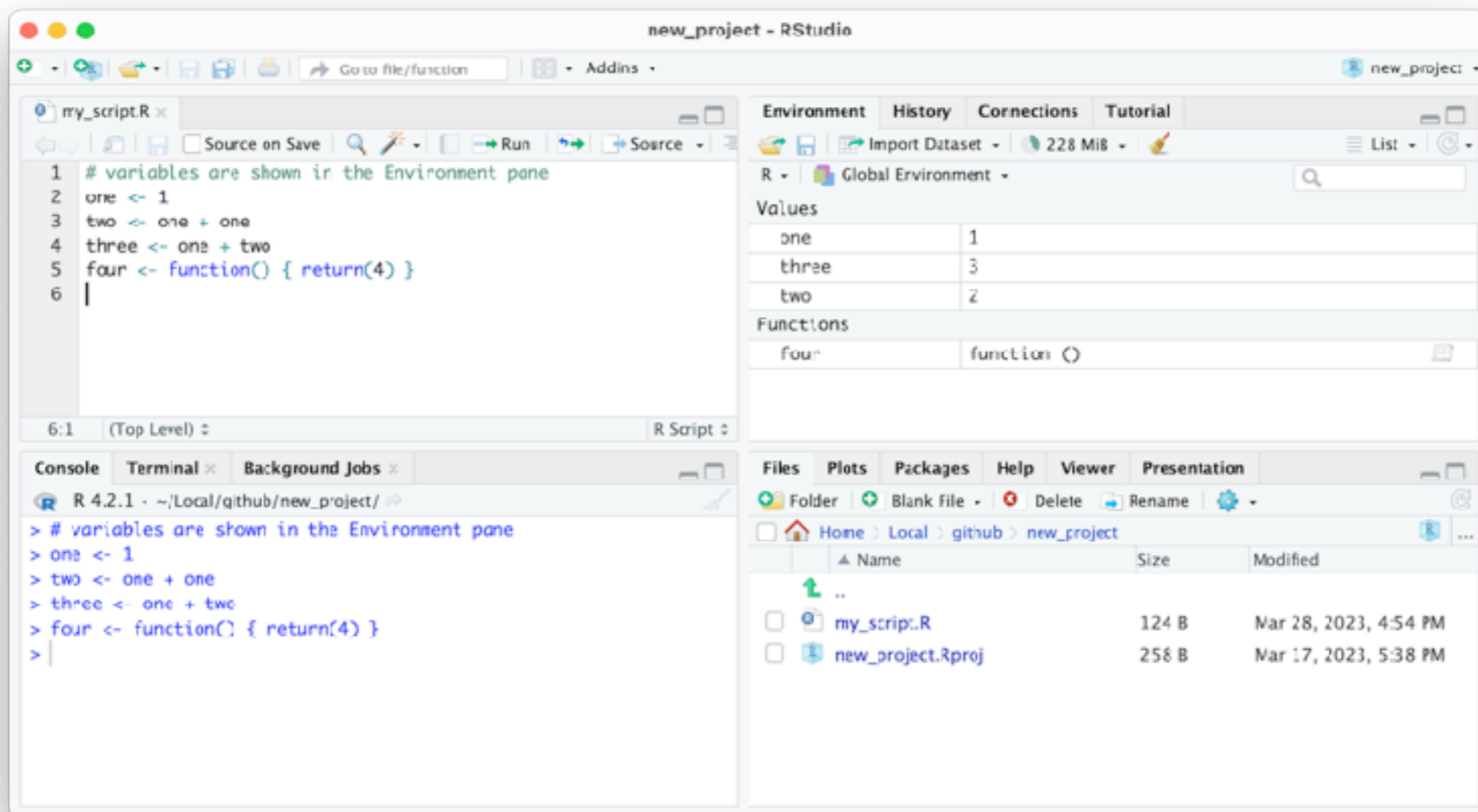
# Why Learn R?

**You choose wisely ... R is a great language for data analysis!**

- Many programming languages are general purpose (can be used in any domain), e.g. C/C++, Java, Python
- R is not a general purpose programming language, it's a language specifically designed for working with data (that's what scientists do!)
- Because R is geared toward data, its design, structure and continued development is focused on making it easier to work with data
- R has become one of the top languages for data science, and it's popularity and usage continues to grow
- For scientists, R is a great tool to learn

# Write Code with *R* and *RStudio IDE*

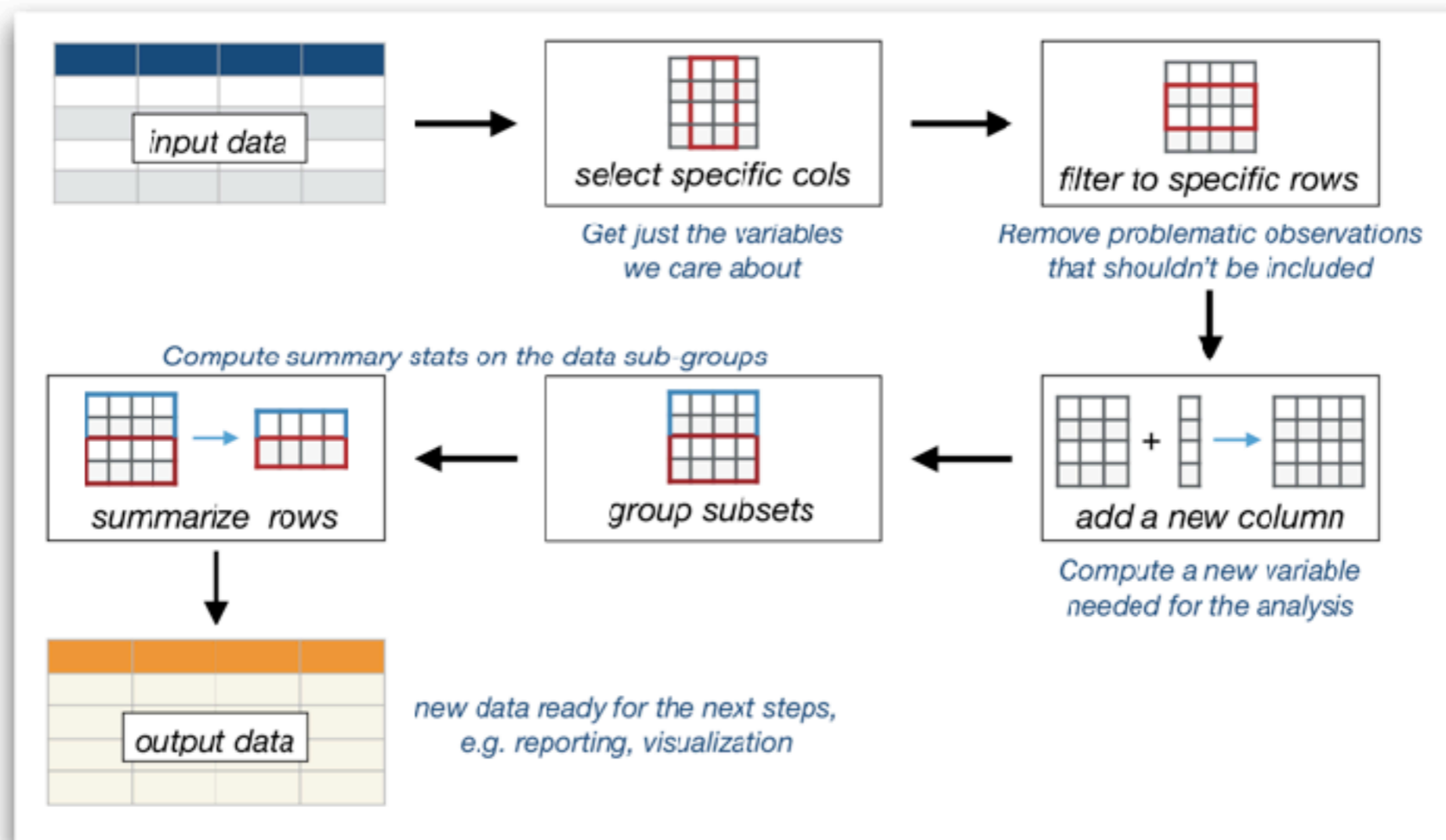
- RStudio provides an integrated development environment (IDE) for coding.
- Streamlines all aspects of the data analysis process.
- Learn best practices for organizing analyses into projects and make your work reproducible.





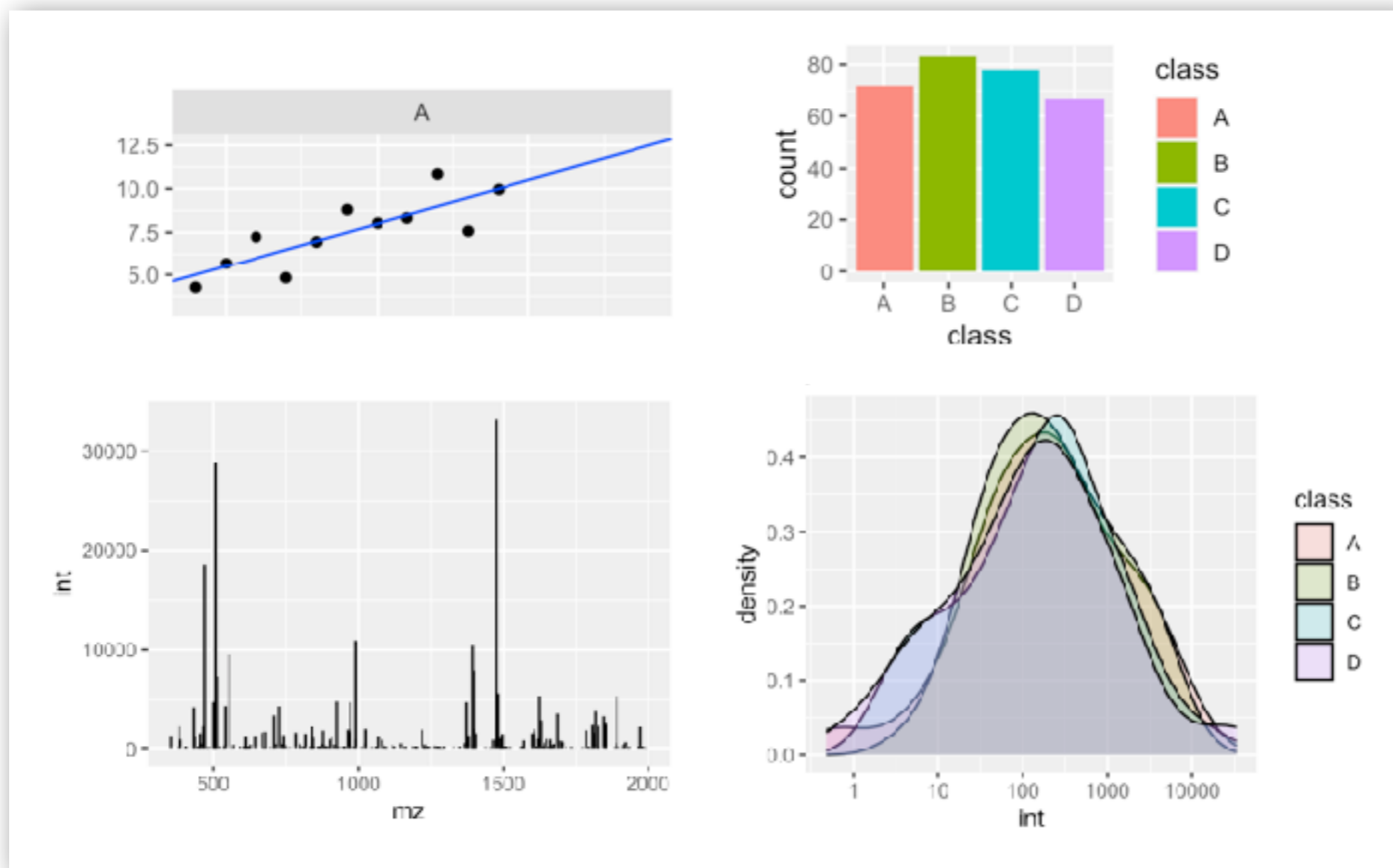
# Organize Data with the *Tidyverse*

- Learn how *clean-up* data and make analysis code easier to read, write and understand.
- The tidyverse covers all steps of the analysis process, from data import & cleaning to visualization and final reporting



# Visualize Data with *GGPlots*

- Learn to visualize data helping to understand patterns, trends, and relationships.
- A well-designed visualization can make complex data easy to understand and convey insights that would be hard to discern from raw data.



# What do we hope to accomplish?

**At the end of the course, you are able to ...**

- start-up R Studio and make an R project.
- read a formatted data file in to R.
- understand basic properties about the data.
- convey what tidy data is and why it is important.
- perform data manipulations, summaries and analyses.
- construct a plot with the data.
- know where to go to expand your knowledge.